Chemical and Bonding State Analysis of As Dopant in Si Semiconductor by XAFS

Doping in silicon semiconductor is an important technique for controlling electronic properties, while chemical and bonding state of dopant element has not been investigated. We are showing chemical, bonding, and coordination analysis of arsenic dopant by XAFS.

1. Sample

Si substate implanted ^{75}As ion
- ✓ w/o anneal (as implanted)
- ✓ w/ anneal (950 °C, 30 min)

Ion Implantation Condition

Substrate	P-type silicon
Energy	200 keV
Dosage	1×10^{15} atoms / cm^2

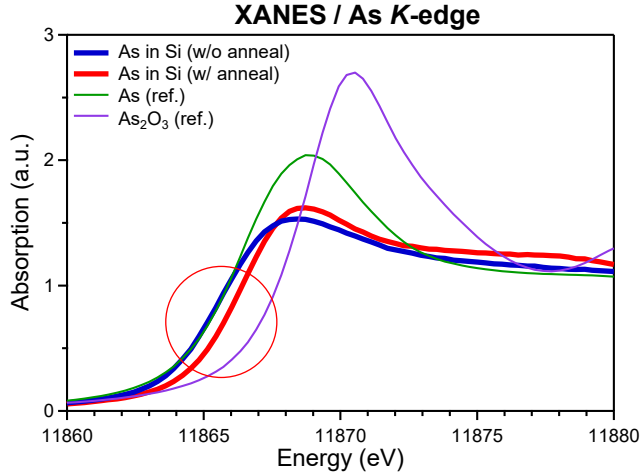
2. Experimental

Synchrotron facility utilization

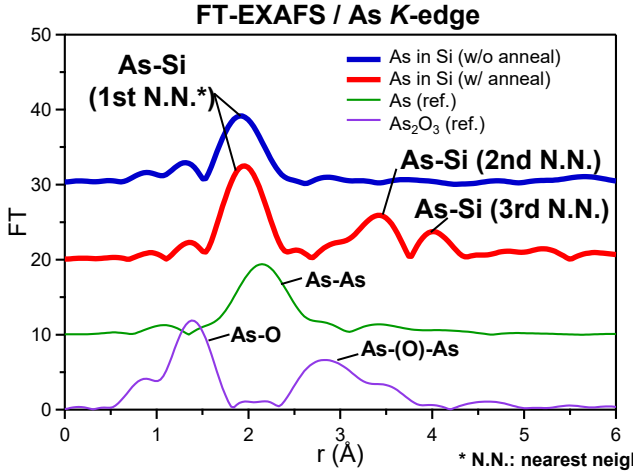
XAFS(X-ray Absorption Fine Structure)
- XANES (X-ray Absorption Near Edge Structure)
  Chemical state analysis
- EXAFS (Extended X-ray Absorption Fine structure)
  Coordination and bonding state analysis
  Radial distribution function (FT-EXAFS)

3. XAFS of As dopant

XANES / As *K*-edge



FT-EXAFS / As *K*-edge



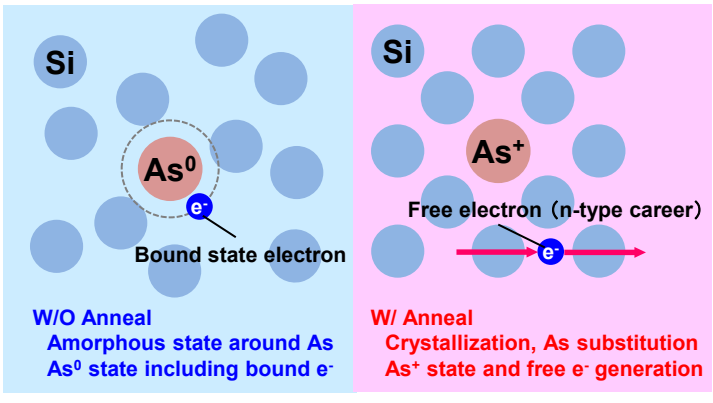
* N.N.: nearest neighbor atom

- ✓ w/o anneal : Agreement wit simple As → As^0
- ✓ w/ anneal : Shift to high energy side → As$^+$

- ✓ W/O Anneal : only As-Si(1st N.N.), Random Coordination
- ✓ W/ Anneal : As-Si(1st, 2nd, 3rd N.N.), High symmetry

Our XAFS analytical service suggests suitable analysis dependent on sample and aim, e.g. high sensitivity measurement and quantitative analysis !

4. Schematic image of As state in Si lattice



Chemical, Bonding, and Coordination state of the Dopant Element can be Examined by XAFS !

5. Structure Parameter from FT-EXAFS

Interatomic Distance and Coordination Number was Estimated by EXAFS Curve Fitting Analysis. **

	W/O Anneal	W/ Anneal		
path	As-Si 1st N.N.	As-Si 1st N.N.	As-Si 2nd N.N.	As-Si 3rd N.N.
R (Å)	2.33	2.35	3.78	4.42
CN	2.9	3.8	6.4	16.8
σ^2 (Å^2)	0.00356	0.00302	0.00412	0.01694
R-factor	0.0176	0.0184		

Annealing increased coordination number of As-Si bonding, and generated 4-folded substituted state in Si crystal lattice.

** R and CN mean interatomic distance and coordination number, respectively. σ^2 is Debye Waller factor, the parameter related with structural order/disorder and thermal oscillation. R-factor dependent on fitting agreement, and the value less than 0.05 represents reasonable optimization.

XAFS analysis of dopant element in silicon or compound semiconductor reveals dopant activation with carrier generation and substitution in matrix lattice, through the investigation of chemical and structural state of dopant element.

P02303表面科学第2研究室20210803

Toray Research Center, Inc.